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The Enumeration of Homeomorphically Irreducible Labelled Graphs

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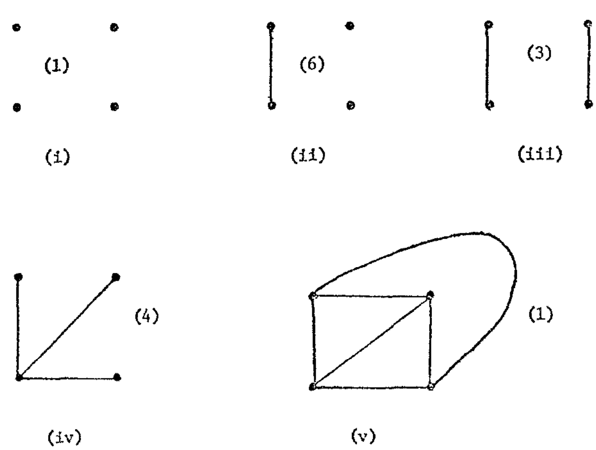
The counting series for homeomorphically irreducible labelled graphs is given. A linear recurrence equation is obtained to facilitate the tabulation of the number of such graphs on a specified number of vertices.

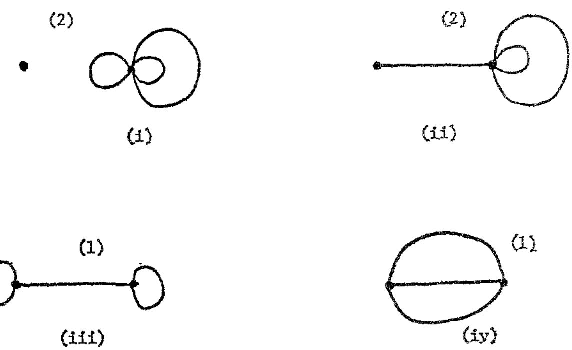
1. INTRODUCTION AND NOTATION

A graph is said to be homeomorphically irreducible if it contains no bivalent vertices. For convenience, we refer to a tree or graph with this property as an *h-tree* or an *h-graph*, respectively. A graph is said to be *simple* if it contains no loops or multiple edges. To fix ideas, the following is a complete enumeration of simple *h*-graphs on 4 vertices.



The parenthetic figure beside each graph gives the number of ways in which the graph may be labelled. Thus, there are 5 *connected simple* *labelled h-graphs* and 15 *simple labelled h-graphs* on 4 vertices. The term *labelling* will be understood to denote vertex labelling.

The following is an enumeration of h-graphs with 3 edges and 2 vertices.



The parenthetic figure beside each graph gives the number of ways in which the graph may be labelled. There are, therefore, 4 *connected labelled h-graphs* and 6 *labelled h-graphs* on 3 edges and 2 vertices.

The enumeration of labelled h-trees is a special case of the *h-graph enumeration problem*, and has been treated by Meir and Moon [1] and, more recently, by Read [2]. The purpose of the present paper is to provide a treatment of the h-graph enumeration problem for simple graphs. Graphs are then treated in a similar fashion. A tabulation for simple labelled h-graphs and connected simple labelled h-graphs is given with respect to the number of vertices to demonstrate that the expressions for the counting series are susceptible to numerical computation. The computations may be reduced to iterating a fourth order linear recurrence equation in two variables.

In the counting series which will be developed the elements x and y are used as *edge-weight* and *vertex-weight*, respectively. The elements are members of a commutative ring. Suppose that $\mathscr{A}$ is a set of labelled graphs and that $a_{p,q}$ is the number of members of $\mathscr{A}$ which have q edges and p vertices. Then we shall refer to

$$A(x, y) = \sum_{p,q} a_{pq} \frac{x^q y^p}{p!}$$

as the *exponential counting series* for the set $\mathscr{A}$ or the *exponential generating function* for the sequence $\{a_{p,q}\}$. The series is exponential only in the labelled elements, namely the vertices, but this usage does not lead to ambiguity.

The counting series for the sets of figures which arise in the combinatorial decomposition of the problem have been constructed by a uniform method in which the combinatorial operations (for example, edge subdivision) are representable directly by algebraic operations on the appropriate counting series. It has therefore been possible to abbreviate several of the proofs of the propositions in which these counting series are stated.

In the subsequent development, we shall have occasion to consider the number of distinguishable configurations among a set S under an equivalence relation E. This number is the cardinality of the quotient set S/E. As a matter of convenient terminology we shall say that the generating function for the set S/E is obtained from the generating function for S by "factoring out" the equivalence relation. This is achieved by certain elementary operations on the terms of a generating function itself, and will be seen in detail later.

The operator $[x^p]$ applied to the function $f(x)$ gives the coefficient of x^p in the Laurent series expansion of $f(x)$ at the origin. The convention is adopted that there is a *null-graph* with no vertices, no edges and no components, which is not connected. The graph theoretic terminology employed in this paper follows the usage of Tutte [3].

2. Homeomorphically Irreducible Trees

We first derive the result obtained by Meir and Moon [1] for the number of labelled h-trees on n vertices. The proof which is given here illustrates the technique which will be used repeatedly in the treatment of labelled h-graphs.

Proposition 1. (Cayley's Formula). *Let $T(y)$ be the exponential counting series for the number of labelled trees. Then*

$$T(y) = \sum_k k^{k-2} \frac{y^k}{k!}.$$

Proof. See, for example, Riordan [4].

Theorem 1. *Let $U(y)$ be the exponential generating function for the number, u_n, of labelled h-trees on n vertices. Then*

$$u_n = (n-2)! \sum_k (-1)^{n-k} \binom{n}{k} \frac{k^{k-2}}{(k-2)!}.$$

Proof. Let s_n be the number of simple connected labelled h-graphs on n

vertices and $n-1$ edges, and let $S(x, y)$ be the exponential generating function for $\{s_n\}$. Since these h-graphs are trees, then

$$S(x, y) = x^{-1}U(xy).$$

Now every tree may be constructed uniquely by subdividing the edges of and h-tree. Moreover, this operation is reversible. But the edge subdivision for each edge is accomplished by the substitution,

$$x = 1 + y + y^2 + \dots = (1 - y)^{-1}.$$

Since the construction is bijective

$$S((1-y)^{-1}, y) = T(y)$$

whence

$$(1-y)\, U(y(1-y)^{-1}) = T(y).$$

This may be inverted by the substitution

$$z = y(1-y)^{-1}$$

to yield

$$U(z) = (1+z)\, T(z(1+z)^{-1})$$

from which the theorem follows by applying $[z^n/n!]$, using Proposition 1.

3. Preliminaries

We obtain the counting series for the number of simple h-graphs by constructing simple graphs which have at least i bivalent vertices and by using the Principle of Inclusion and Exclusion. Graphs with the above property are constructed from the sets of graphs $\mathscr{C}$ (circuits), $\mathscr{M}$ (multiple edge, with subdivision) and $\mathscr{L}$ (multiple loop, with subdivision), since these are the only sets of figures in which bivalent vertices may reside. The exponential counting series for these sets are given in the following propositions.

Proposition 2. *Let $\mathscr{C}$ be the set of labelled simple graphs whose components are circuits. Let $c_{p,q}$ be the number of such graphs with q edges and p vertices. Then the exponential generating function for $\{c_{p,q}\}$ is*

$$C(x, y) = (1 - xy)^{-1/2} \exp\left(-\frac{xy}{2} - \frac{x^2y^2}{4}\right).$$

Proof. The exponential counting series for plane rooted labelled circuits is

$$x^3y^3 + x^4y^4 + \dots.$$

The terms 1, xy and x^2y^2 have been omitted since they correspond to the null circuit, the loop and a multiple edge, respectively. The exponential counting series for the abstract graph corresponding to the circuits enumerated by this series is obtained by factoring out the dihedral operation. This yields

$$\tfrac{1}{2}(x^3y^3 + x^4y^4 + \cdots).$$

The rooting is abolished by factoring out the cyclic rotation. The exponential counting series for labelled circuits is accordingly

$$\frac{1}{2}\left(\frac{x^3y^3}{3} + \frac{x^4y^4}{4} + \cdots\right).$$

The exponential counting series for labelled simple graphs whose components are circuits is

$$\exp \frac{1}{2}\left(\frac{x^3y^3}{3} + \frac{x^4y^4}{4} + \cdots\right).$$

Thus

$$C(x, y) = (1 - xy)^{-1/2} \exp\left(-\frac{xy}{2} - \frac{x^2y^2}{4}\right).$$

PROPOSITION 3. *Let $\mathscr{M}$ be the set of simple connected labelled graphs constructed on a multiple edge by edge subdivision. Let $m_{p,q}$ be the number of such graphs, with q edges and p bivalent vertices. Then the exponential generating function for $\{m_{p,q}\}$ is*

$$M(x, y) = (1 + x) \exp\left(\frac{x^2y}{1 - xy}\right).$$

Proof. Each member of $\mathscr{M}$ is homeomorphically reducible to a graph on two vertices. We shall call these vertices the distinguished vertices. Suppose there is no edge connecting the distinguished vertices. Then each edge of the multiple edge is distinguishable from the others because of the labels attached to the vertices to be inserted in each of the edges. Suppose that the distinguished vertices are m-valent. The exponential counting series for the distinguishable multiple edges embedded in the plane is

$$x^m.$$

The exponential counting series for the corresponding abstract graph is obtained by factoring out the symmetric group. This yields

$$x^m/m!.$$

The exponential counting series for multiple edges is accordingly the sum of these, namely,

$$E(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \cdots = \exp x.$$

Now each edge may be subdivided. The counting series for edge subdivision is

$$x^2y + x^3y^2 + \cdots = x^2y(1 - xy)^{-1}.$$

Thus the exponential counting series for the members of $\mathscr{M}$ with no edges joining the distinguished vertices is

$$E(x^2y(1 - xy)^{-1}) = \exp(x^2y(1 - xy)^{-1}).$$

The excluded case, namely a simple edge joining the distinguished vertices, is counted by

$$1 + x.$$

Thus

$$M(x, y) = (1 + x) \exp\left(\frac{x^2y}{1 - xy}\right).$$

PROPOSITION 4. *Let $\mathscr{L}$ be the set of simple connected labelled graphs consisting of multiple loops with edge subdivision. Let $l_{p,q}$ be the number of such graphs with q edges and p bivalent vertices. Then the exponential generating function for $\{l_{p,q}\}$ is*

$$L(x, y) = \exp\left(\frac{\frac{1}{2}x^3y^2}{1 - xy}\right).$$

Proof. Similar to Proposition 3.

4. SIMPLE GRAPHS

The main result gives the exponential counting series for simple labelled h-graphs. The result is obtained by constructing a graph on n vertices which has at least i bivalent vertices, and by applying inclusion and exclusion.

THEOREM 2. *Let $H(x, y)$ be the exponential generating function for the number $h_{p,q}$ of simple labelled h-graphs on q edges and p vertices. Then*

$$H(x, y) = (1 + xy)^{-1/2} \exp\left(\frac{xy}{2} - \frac{x^2y^2}{4}\right)$$

$$\times \sum_{j=0}^{\infty} \frac{1}{j!} \left\{(1 + x) \exp\left(\frac{-x^2y}{1 + xy}\right)\right\}^{\binom{j}{2}} \left\{y \exp\left(\frac{\frac{1}{2}x^3y^2}{1 + xy}\right)\right\}^j.$$

Proof. Consider a set π of n labelled vertices. Select a subset σ of π with i vertices. A subset ρ of π remains with $j = n - i$ vertices. On π construct a graph in which every vertex in σ is bivalent, as follows. Consider the set ρ of vertices. Between each distinct pair of vertices of ρ insert a member of $\mathscr{M}$, with bivalent vertices taken from σ. At each vertex of ρ attach a member of $\mathscr{L}$ with bivalent vertices taken from σ. Assign the remaining vertices of σ among the members of $\mathscr{C}$. The sum of graphs on n vertices, m edges and having the subset σ as bivalent vertices is

$$\binom{n}{j} \alpha_{mi}$$

where

$$\alpha_{mi} = \left[x^m \frac{y^i}{i!}\right] C(x, y)(M(x, y))^{\binom{j}{2}} (L(x, y))^j.$$

The term $\binom{n}{j}$ is the number of ways labels may be assigned to ρ. Note that there may be more than i bivalent vertices since a bivalent vertex may arise by the insertion of an edge between vertices which are univalent. By the Principle of Inclusion and Exclusion, the number of simple labelled h-graphs with n vertices and m edges is

$$\sum_i \binom{n}{i} (-1)^i \alpha_{mi} = \left[x^m \frac{y^n}{n!}\right] \sum_j \frac{y^j}{j!} C(x, -y)(M(x, -y))^{\binom{j}{2}}(L(x, -y))^j$$

and the theorem follows from Propositions 2, 3, and 4.

COROLLARY 1. *The generating function for the number $h^*_{p,q}$ of connected simple labelled h-graphs on q edges and p vertices is*

$$H^*(x, y) = \log H(x, y).$$

Proof. Application of a theorem of Gilbert [5].

COROLLARY 2. *The exponential generating function for the number h_p of simple labelled h-graphs on p vertices is*

$$h(y) = (1+y)^{-1/2} \exp\left\{\frac{y}{2} - \frac{y^2}{4}\right\}$$
$$\times \sum_{j=0}^{\infty} y^j \frac{2^{\binom{j}{2}}}{j!} \exp\left(\frac{-\frac{1}{2}j(j-1)y + \frac{1}{2}jy^2}{1+y}\right).$$

Proof. Direct from Theorem 2, putting $x = 1$.

5. EXTENSION TO GRAPHS

The result may be extended in a straightforward manner to graphs. The same construction may be employed but the sets $\mathscr{C}$, $\mathscr{M}$ and $\mathscr{L}$ must be augmented by multiple edges and loops as appropriate, to become $\mathscr{C}^+$, $\mathscr{M}^+$ and $\mathscr{L}^+$. The following propositions give the definitions of these sets together with the appropriate generating functions.

PROPOSITION 5. *Let $\mathscr{C}^+$ be the set of labelled graphs whose components are circuits. Let $c^+_{p,q}$ be the number of such graphs with q edges and p vertices. Then the exponential generating function for $\{c^+_{p,q}\}$ is*

$$C^+(x, y) = (1 - xy)^{-1/2} \exp\left(\frac{xy}{2} + \frac{x^2y^2}{4}\right).$$

Proof. The proof is similar to Proposition 2.
The contribution from the circuit and the loop is

$$xy + \tfrac{1}{2}x^2y^2.$$

The exponential counting series for labelled graphs whose components are circuits is

$$\exp\left(xy + \frac{1}{2}x^2y^2 + \frac{1}{2}\left(\frac{x^3y^3}{3} + \frac{x^4y^4}{4} + \cdots\right)\right).$$

Thus

$$C^+(x, y) = (1 - xy)^{-1/2} \exp\left(\frac{1}{2}xy + \frac{x^2y^2}{4}\right).$$

PROPOSITION 6. *Let $\mathscr{M}^+$ be the set of labelled connected graphs constructed on a multiple edge by edge subdivision. Let $m^+_{p,q}$ be the number of* *such graphs with q edges and p bivalent vertices. Then the exponential generating function for $\{m^+_{p,q}\}$ is*

$$M^+(x, y) = (1 - x)^{-1} \exp\left(\frac{x^2y}{1 - xy}\right).$$

Proof. Similar to Proposition 3. The series $(1 - x)^{-1}$ replaces $(1 + x)$ and enumerates the multiple edges.

PROPOSITION 7. *Let $\mathscr{L}^+$ be the set of labelled connected graphs consisting of multiple loops with edge subdivision. Let $l_{p,q}$ be the number of such graphs with q edges and p bivalent vertices. Then the exponential generating function for $\{l^+_{p,q}\}$ is*

$$L^+(x, y) = (1 - x)^{-1} \exp x^2y \exp\left(\frac{\frac{1}{2}\, x^3y^2}{1 - xy}\right).$$

Proof. The proof is similar to Proposition 3. The series $(1 - x)^{-1}$ enumerates the multiple loops. The series $\exp x^2y$ enumerates loops with a single vertex inserted by edge subdivision. The figure is invariant under the dihedral operation, so lacks the factor of $\frac{1}{2}$.

THEOREM 3. *Let $H^+(x, y)$ be the exponential generating function for the number, $h^+_{p,q}$, of labelled h-graphs on q edges and p vertices. Then*

$$H^+(x, y) = (1 + xy)^{-1/2} \exp\left(-\frac{xy}{2} + \frac{x^2y^2}{4}\right)$$
$$\times \sum_{j=0}^{\infty} \frac{y^j}{j!}(1-x)^{\frac{-j(j+1)}{2}}\left(\exp\frac{-x^2y}{1+xy}\right)^{\binom{j}{2}}\left\{\exp\left(-x^2y+\frac{\frac{1}{2}\,x^3y^2}{1+xy}\right)\right\}^j.$$

Proof. Similar to Theorem 2, replacing $C(x, y)$, $M(x, y)$ and $L(x, y)$ by $C^+(x, y)$, $M^+(x, y)$ and $L^+(x, y)$.

6. COMPUTATIONAL SCHEME

A scheme for computing the number h_n of simple labelled h-graphs on n vertices is provided by the following corollary.

COROLLARY 3.

$$h_n = n! \sum_{j=0}^{n} \frac{1}{j!}\, 2^{\binom{j}{2}} a^{(j)}_{n-j}$$

where $\{a_k^{(j)}\}$ *satisfies the linear recurrence equation*

$$2(k+1)\,a_{k+1}^{(j)} = (j - j^2 - 4k)\,a_k^{(j)} + 2(1+j-k)\,a_{k-1}^{(j)} + (j-1)\,a_{k-2}^{(j)} - a_{k-3}^{(j)}$$

with initial conditions

$$\begin{aligned} a_0^{(j)} &= 1, \\ a_1^{(j)} &= -\frac{1}{2}\,j(j-1), \\ a_2^{(j)} &= \frac{1}{8}\,j^2(j^2-2j+5), \\ a_3^{(j)} &= -\frac{1}{48}(j^6 - 3j^5 + 15j^4 - 13j^3 + 24j^2 + 8). \end{aligned}$$

Proof. From Corollary 2 we have

$$h(y) = \sum_{j=0}^{\infty} \frac{y^j}{j!}\, 2^{\binom{j}{2}} g_j(y)$$

where

$$\begin{aligned} g_j(y) &= (1+y)^{-1/2} \exp\left(\frac{y}{2} - \frac{y^2}{4}\right) \cdot \exp\left(\frac{-\frac{1}{2}j(j-1)\,y + \frac{1}{2}jy^2}{1+y}\right) \\ &= \exp\left\{-\frac{1}{2}\log(1+y) + \frac{1+j}{2}\,y - \frac{y^2}{4} - \frac{j^2}{2}\frac{y}{1+y}\right\}. \end{aligned}$$

Differentiating logarithmically with respect to y we have

$$2(1+y)^2 g_j'(y) + \{(1+y)^2 y + j^2 - (1+y)^2(1+j) - (1+y)\}\, g_j(y) = 0$$

so

$$2(1+y)^2 g_j'(y) + \{(1+y)\,y^2 + j^2 - j(1+y)^2\}\, g_j(y) = 0$$

Let

$$g_j(y) = \sum_{k=0}^{\infty} a_k^{(j)} y^k.$$

The recurrence equation is obtained by comparing coefficients of y^k. The initial conditions may be obtained by expanding $g_j(y)$ to the cubic term in y by Maclaurin's Theorem.

Corollary 3 implies that the time taken to compute h_n is $O(n^2)$ The same device may be used to provide a numerical scheme for computing the coefficients of $H(x, y)$ and $H^+(x, y)$.

COROLLARY 4. *Let $h_n{}^*$ be the number of connected simple labelled h-graphs on n vertices. Then*

$$h_{k+2}^* = \frac{1}{k+2}\left(h_k - \sum_{j=0}^{k+1} j h_j{}^* h_{k+2-j}\right).$$

Proof. Let $h^*(y)$ be the exponential generating function for $\{h_n^*\}$. Then, from Corollary 1 and Corollary 2,

$$h^*(y) = \log h(y).$$

Thus

$$(h^*(y))' \, h(y) = h'(y).$$

The result follows by comparing coefficients.

Corollary 4 implies that the time taken to compute h_n^* is $O(n^2)$.

TABLE I

The Number of Simple Labelled *h*-Graphs on *n* Vertices

n	Number of Graphs
0	1
1	1
2	2
3	4
4	15
5	102
6	4166
7	402631
8	76374899
9	27231987762
10	18177070202320
11	22801993267433275
12	54212469444212172845
13	24681269732651812735138 4
14	21737873047967352627094193 50
15	37373588848096468764431235680525
16	126351353411060614102667677842203156 1
17	844613956864436221035392666142771505959 00
18	112076711834706844779379655344355968945740335 20
19	296024078194738729505593525089159922734781161147555 5
20	15590900691712854279344433528640836723800930638494654902 59

7. Tabulated Values

The following Tables I and II, give the numbers of simple labelled h-graphs and connected simple labelled h-graphs on a specified number of vertices. The tables were computed by expanding $h(y)$ and $\log h(y)$ up to y^{20} using the algebraic manipulation language ALTRAN, on a Honeywell 6050 Computer.

Table III gives the number of simple labelled h-graphs on q edges and p vertices in both the connected and unrestricted cases. It should be noted that the number of labelled h-trees, enumerated by Theorem 1, appears as the superdiagonal $\{h^*_{p-1,p}\}$ of this table.

TABLE II

The Number of Simple Labelled Connected h-Graphs on n Vertices

n	Number of Graphs
0	0
1	1
2	1
3	0
4	5
5	51
6	3634
7	374119
8	73161880
9	26545249985
10	17904840957826
11	22602069719494379
12	53938847227326533032
13	246107945479472758874483
14	2170331943503938546383205218
15	37340982087637629911717846092591
16	1262915556964772342158139988356979872
17	84439915959315968795939888804062790596833
18	11206150878409275555887475857385649197136029346
19	2960027836197349026427594597111901309290325827539367
20	155903086435583900939981739181924750313325299309288235 0248

TABLE III

Number of Simple Labelled $\begin{Bmatrix} \text{Connected} \\ \text{Unrestricted} \end{Bmatrix}$ h-Graphs on q Edges and p Vertices

h	p	0	1	2	3	4	5	6	7	8
0		0	1	0	0	0	0	0	0	0
		1	1	1	1	1	1	1	1	1
1				1	0	0	0	0	0	0
				1	3	6	10	15	21	28
2						0	0	0	0	0
						3	15	45	105	210
3						4	0	0	0	0
						4	20	75	245	700
4						0	5	0	0	0
						0	5	90	525	2065
5						0	0	96	0	0
						0	0	96	777	4368
6						1	0	120	427	0
						1	5	135	1302	10094
7							20	180	1260	6448
							20	315	3045	26468
8							15	420	3780	23520
							15	510	7455	74970
9							10	700	10850	79800
							10	760	16275	201320
10							1	837	24045	269360
							1	843	30135	506492
11								765	44814	782880
								765	50190	1186416
12								395	68040	1956136
								395	70805	2532971
13								105	80955	4203360
								105	81690	4865000
14								15	70500	7610340
								15	70605	8177700
15								1	43232	11365676
								1	43239	11711980

Table continued

TABLE III (*continued*)

h	p	0	1	2	3	4	5	6	7	8
16									18774 18774	13652835 13803055
17									5880 5880	12987408 13034448
18									1330 1330	9789346 9799986
19									210 210	5906040 5907720
20									21 21	2884497 2884665
21									1 1	1148752 1148760
22										373212 373212
23										98112 98112
24										20475 20475
25										3276 3276
26										378 378
27										28 28
28										1 1

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